Indian J. Phys. **78(8)**, 809-814 (2004)

AN INTERNATIONAL JOURNAL
IJP

The spin-density-wave (SDW) in quaternary borocarbide superconductors

K C Bishoyi[1]*, G C Rout[2] and S N Behera[3]
[1]P G Department of Physics, F M College (Autonomous), Balasore-756 001, Orissa, India
[2]Condensed Matter Physics Group, Government Science College, Chatrapur-761 020, Orissa, India
[3]Institute of Physics, Sachivalaya Marg, Bhubaneswar-751 005, Orissa, India

E-mail : bishoyi@iopb.res.in

Abstract : A large family of quaternary borocarbides RNi_2B_2C (R = Lu, Y, Ho, Dy) was discovered which have separate phase of anti-ferromagnetism (AFM), superconductivity (SC) and co existent anti-ferromagnetic superconductivity. We propose a spin-density-wave (SDW) state as a possible mechanism of the anomalours anti-ferromagnetism in the borocarbide superconductors. In this SDW state, the electron-hole pair amplitude changes its sign in the momentum space The BCS type mean field superconductivity and a mean field SDW in Hubbard model are considered. The superconducting gap and SDW gap are calculated by Zubarev's technique of equation of motion method and are solved self-consistently for different model parameters. The co-existence of superconductivity and anti-ferromagnetism for both of the cases *i.e.* $T_c > T_N$ and $T_c < T_N$ are explained.

Keywords : Quaternary borocarbides, spin density waves.

PACS Nos. : 74.70.Dd, 75.30.Fv

1. Introduction

It is well known that the spin density wave (SDW) and superconductivity (SC) co-exist in a variety of systems, *e.g.* the co-existence is well documented in the itinerant anti-ferromagnetic metal Cr and its alloys [1], organic layered superconductors, the Bechgaard salts (TMTSF)X, with X = PF_6, AsF_6 and ClO_4 [2] and heavy fermion systems URu_2Si_2 and $U_{1-x}Th_xBe_{13}$ [3]. It is observed that URu_2Si_2, UNi_2Al_3 and UPd_2Al_3 compounds are SDW super-conductors but with different degrees of magnetic moment localization. All these systems have a low dimensional structure and exhibit Fermi surface instabilities which drive the SDW transition. One can tentatively add to these classes of materials, the high-T_c perovskite oxide superconductors, $La_{2-x}Sr_xCuO_4$ and $YB_2Cu_3O_{7-\delta}$ which have two dimensional structures and inhibit anti-ferromagnetic order [4], as the probable candidates for the co-existence of SDW and SC. In these correlated superconductors, the porbability of co-existence of SDW and SC has been demostrated [5] at the mean field level.

Recently, the large family of quaternary borocarbides was discovered, which have separate phases of anti-ferromagnetism (AFM), SC and coexisting AFM superconductivty [6–10]. It is possible to study the interplay of AFM and SC for both the cases, $T_c > T_N$ and $T_c < T_N$. Incommensurate magnetic structures (SDWs) with the wave vector ($\simeq$ 0.55, 0, 0), originating from the Fermi surface nesting are found for $LuNi_2B_2C$ [11–13], YNi_2B_2C [12], $TbNi_2B_2C$ [14], $ErNi_2B_2C$ [10,15,16], $HoNi_2B_2C$ [10,17], $GdNi_2B_2C$ [18] and with wave vector ($\simeq$ 0.093, 0.093, 0) for $TmNi_2B_2C$ [10]. It is natural to make an extrapolation that other members of the family may possess the same property. Especially interesting is the situation in $HoNi_2B_2C$ with $T_N \sim 8.5$ K and $T_c \sim 8.0$ K [10]. Here, superconductivity tends to be almost re-entrant near 5 K, which is revealed by the critical field H_{c2} measurement.

In view of the simultaneous presence of the SDW and SC states in these wide class of metals, it is but natural to enquire as to how the properties of each of the

*Corresponding Author

individual phases become modified due to the presence of the other. In Section 2 of this paper, we formulate the mean field theory of the coexistent, SDW-SC phase. In Section 3, the single particle Green's functions and the corresponding gap equations of the SDW and SC order parameters are obtained by equations of motion method of Zubarev [19]. The interplay of SDW and SC parameters further establish the fact that the two states tend to inhibit each other. The SDW and SC coupled gap equations are solved self-consistently and the results are discussed in Section 4. In the concluding Section 5, attempts are made to correlate the results of this calculation to those observed by experiments in borocarbide systems.

2. Formalism

In case of a correlated system, the SDW state arises due to the repulsive intratomic (Hubbard) Coulomb repulsion (U) between the electrons, driven by a Fermi surface instability. This arises predominantly due to the existence of nested pieces of Fermi surface with electron-hole symmetry given by

$$\epsilon_{k+Q} = -\epsilon_k, \tag{1}$$

where Q is the SDW wave vector equal to twice the Fermi wave vector in a particular direction and ϵ_k is the electron energy. This nesting property is a manifestation of the low dimensionality of the system. If nesting is not perfect then the Fermi surface is only partially destroyed due to the appearance of the SDW gap ($2G$). This allows for the possibility of occurrence of a superconducting instability provided there is an effective attractive interaction between the electrons. A mean field Hamiltonian can be constructed for the SDW state arising from the Hubbard Hamiltonian [20]. Similarly we assume that the SC state is described by the BCS reduced Hamiltonian, where the effective interactive interaction between electrons is produced by the suitable exchange of an excitation which gives rise to the high transition temperature as shown by the authors [21] Behera *et al* have studied the phonon response of the high temperature superconductors in the co-existence of SC and SDW phase [22]. Recently Rout *et al* [23] reported a model study of borocarbide system describing the co-existence of the SC and AFM in presence of hybridization. The mean field Hamiltonian describing the coexistent SDW-SC state is given by

$$H = \sum_{k,\sigma} \epsilon_k C^\dagger_{k,\sigma} C_{k,\sigma} + G \sum_k \left(C^\dagger_{k+Q\uparrow} C_{k\downarrow} + C^\dagger_{k\downarrow} C_{k+Q\uparrow} \right)$$

$$+ \Delta \sum_k \left(C^\dagger_{k\uparrow} C^\dagger_{-k\downarrow} + C_{-k\downarrow} C_{k\uparrow} \right), \tag{2}$$

where $C_{k\sigma}\left(C^\dagger_{k\sigma}\right)$ are the annihilation (creation) operators for the electrons of the nickel atom and ϵ_k is the kinetic energy of the electron with momentum k and spin σ. The G and Δ are the SDW and SC order parameters given by

$$G = -U \sum \left\langle C^\dagger_{k+Q\uparrow} C_{k\downarrow} \right\rangle, \tag{3}$$

$$\Delta = -V \sum \left\langle C^\dagger_{k\uparrow} C^\dagger_{-k\downarrow} \right\rangle, \tag{4}$$

with U and V being respectively the repulsive Coulomb and attractive interaction strengths.

3. Calculation of gap equation

In order to determine the gap equations, the following four Green's functions are defined in terms of electron operators as

$$G_1(k,\omega) = \left\langle\left\langle C_{k\uparrow};\ C^\dagger_{k\uparrow} \right\rangle\right\rangle_\omega,$$

$$G_2(k,\omega) = \left\langle\left\langle C_{-k,Q\downarrow};\ C^\dagger_{k\uparrow} \right\rangle\right\rangle_\omega,$$

$$G_3(k,\omega) = \left\langle\left\langle C_{-k\downarrow};\ C^\dagger_{k\uparrow} \right\rangle\right\rangle_\omega,$$

$$G_4(k,\omega) = \left\langle\left\langle C^\dagger_{-k+Q\uparrow};\ C^\dagger_{k\uparrow} \right\rangle\right\rangle_\omega. \tag{5}$$

The coupled Green's functions are evaluated explicitly by using the Hamiltonian given in eq. (2) using Zubarev's equation of motion method [19].

$$(\omega - \epsilon_k) G_1(k,\omega) = \frac{1}{2\pi} + G G_2(k,\omega) + \Delta G_3(k,\omega),$$

$$(\omega + \epsilon_k) G_2(k,\omega) = G G_1(k,\omega) - \Delta G_4(k,\omega),$$

$$(\omega + \epsilon_k) G_3(k,\omega) = G_4(k,\omega) + \Delta G_1(k,\omega),$$

$$(\omega + \epsilon_k) G_4(k,\omega) = -G G_3(k,\omega) - \Delta G_2(k,\omega). \tag{6}$$

In order to determine the gap eqs. (3) and (4) for the SDW and SC states respectively, it is necessary to evaluate the Green's functions. The above coupled equations are solved to get these Green's functions which are given below.

$$G_1(k,\omega) = \frac{(\omega^2 - E_k^2)(\omega + \epsilon_k)}{2\pi|D(\omega)|}$$

$$G_2(k,\omega) = \frac{G(\omega^2 - e_{2k}^2)}{2\pi|D(\omega)|}$$

$$G_3(k,\omega) = \frac{\Delta(\omega^2 - e_{1k}^2)}{2\pi|D(\omega)|}$$

$$G_4(k,\omega) = \frac{-2G\Delta(\omega - \epsilon_k)}{2\pi|D(\omega)|} \tag{7}$$

where

$$|D(\omega)| = (\omega^2 - E_{1k}^2)(\omega^2 - E_{2k}^2),$$

$$E_{1k} = \sqrt{\epsilon_k^2 + \Delta_1^2}\,, \quad E_{2k} = \sqrt{\epsilon_k^2 + \Delta_2^2}\,, \quad \Delta_{1,2} = (\Delta \pm G),$$

$$e_{1k} = \sqrt{\epsilon_k^2 + \Delta_1\Delta_2}\,, \quad e_{2k} = \sqrt{\epsilon_k^2 - \Delta_1\Delta_2}\,,$$

$$E_k = \sqrt{\epsilon_k^2 + \Delta^2 + G^2}\,. \tag{8}$$

The expressions for the order parameters G and Δ defined by eqs. (3) and (4), are calculated from Green's functions $G_2(\omega)$ and $G_3(\omega)$ respectively. After simplification, those are written as

$$\Delta = \frac{\lambda_1}{4}\int_{-\omega_D}^{+\omega_D} d\epsilon_k \Delta\left[\frac{\Delta_1}{E_{1k}}\tanh\left(\frac{\beta E_{1k}}{2}\right) + \frac{\Delta_2}{E_{2k}}\tanh\left(\frac{\beta E_{2k}}{2}\right)\right. \tag{9}$$

and

$$G = \frac{\lambda_2}{4}\int_{-\frac{W}{2}}^{+\frac{W}{2}} d\epsilon_k G\left[\frac{\Delta_1}{E_{1k}}\tanh\left(\frac{\beta E_{1k}}{2}\right) - \frac{\Delta_2}{E_{2k}}\tanh\left(\frac{\beta E_{2k}}{2}\right)\right], \tag{10}$$

where $\lambda_1 = N(0)$ and $\lambda_2 = N(0)U$ are the dimensionless SC and SDW coupling constants respectively with $N(0)$ being the density of states at the Fermi level. Further more, the cut off energy E_s of the SDW state is defined as the energy above the Fermi energy which destorys the nesting of the Fermi surface completely. Similarly ω_D is the highest frequency of the boson whose exchange brings about the attractive interaction between the electrons. All the quantities entering eqs. (9) and (10) are made dimensionless after dividing those by ω_D. Thus the dimensionless order parameters are redefined as $\Delta/\omega_D = z$ and $G/\omega_D = g$, the variables as $\epsilon_k/\omega_D = x$, $k_BT/\omega_D = t$, $W/\omega_D = \tilde{W}$.

4. Results and discussion

There is a family of borocarbide superconductors where the Néel temperature T_N is greater than the superconducting transition temperature T_c. There is also another family of this system where $T_N < T_c$. To discuss our theoretical model for these two families of borocarbide system, we have selected two sets of coupling constants, one for the SC (*i.e.* λ_1) and another for magnetism (*i.e.* λ_2). The interplay between the SC and the SDW states is discussed below on the basis of our model.

(A) Case $T_N < T_c$:

The temperature dependences of the SC order parameter $z(t)$ for the SC coupling constant $\lambda_1 = 0.238605$ and the SDW order parameter $g(t)$ for the SDW coupling constant $\lambda_2 = 0.130362$ are shown in Figure 1.

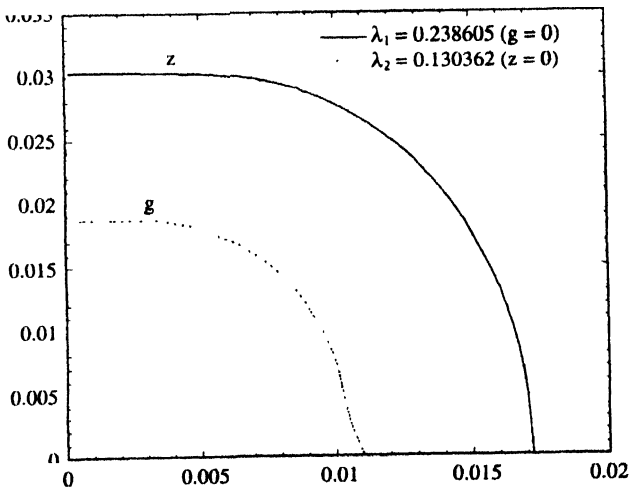

Figure 1. The plot of z *vs* t for fixed values of $g = 0$, $\lambda_1 = 0.238605$, $\lambda_2 = 0$ and the plot of g *vs* t for fixed values of $z = 0$, $\lambda_1 = 0$, $\lambda_2 = 0.130362$.

This choice of coupling constants corresponds to the systems with $T_N > T_c$. The two individual parameters $z(t)$ and $g(t)$ in absence of each other exhibit usual BCS like mean-field temperature dependence. The SC transition temperature $t_c \simeq 0.017$ and the SC gap $z(t = 0) \simeq 0.03$ which corresponds to $2\Delta(0)/k_BT_c \simeq 3.52$. Similarly the SDW system gives a Néel temperature $t_N \simeq 0.011$ and $g(t = 0) \sim 0.019$. Since the long range orders are present

simultaneously *i.e.* for the case of co-existence of SC and SDW, the eqs. (9) and (10) are solved self-cosnsistently for the same values of coupling constant as shown in Figure 2.

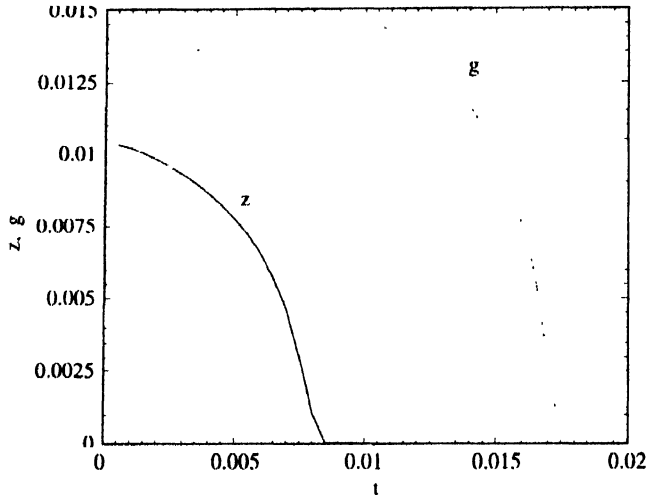

Figure 2. The self-consistent plot of z, g *vs* t for fixed values of $\lambda_1 = 0.238605$, $\lambda_2 = 0\ 130362$.

In the co-existent phase, both the SC and SDW states are suppressed considerably. However, even though the coupling constants are same, the SDW transition temperature t_N is greatly enhanced as if the roles of the SC and the SDW are reversed with $t_N > t_c$ as shown in Figure 2. This situation depicts a similar situation $t_N > t_c$ observed in boracarbide system $DyNi_2B_2C$ with $T_N = 10$ K and $T_c = 6$ K. The SC order parameter shows a mean field behaviour with the value $2\Delta/k_BT_c$ ~2.66 which is slightly less than the universal BCS constant. The SDW order parameter at the outset increases as the temperature is lowered below t_N, attains a maximum around $t_N/2$ and then starts decreasing at the onset of SC *i.e.* in the temperature range $t < t_c$.

The effect of SC coupling constant λ_1 on SC order parameter $z(t)$ and SDW order parameter $g(t)$ is shown in Figure 3. The increase in SC coupling constant λ_1 decreases the SC order parameter and pushes the transition temperature t_c to lower temperatures. However, the parameter $z(t = 0)$ remains unaltered with change in value of λ_1. This contradicts the BCS type behaviour. It is obtained that the SDW gap $g(t)$ increases throughout the temperature range with increase of λ_1. But the Néel temperature (t_N) is enhanced in the co-existent phase.

The effect of SDW coupling constant λ_2 on SC gap parameter $z(t)$ and the SDW gap parameter $z(t)$ in co-existent phase is shown in Figure 4.

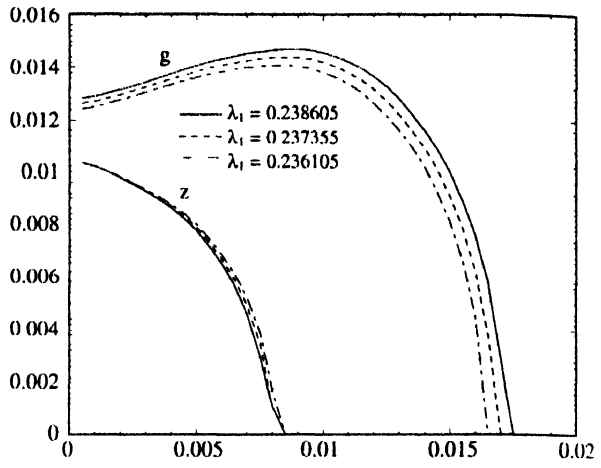

Figure 3. The self-consistent plot of z, g *vs* t for fixed value of $\lambda_2 = 0.130362$ and for different values of $\lambda_1 = 0.238605$, 0 237355, 0.236105.

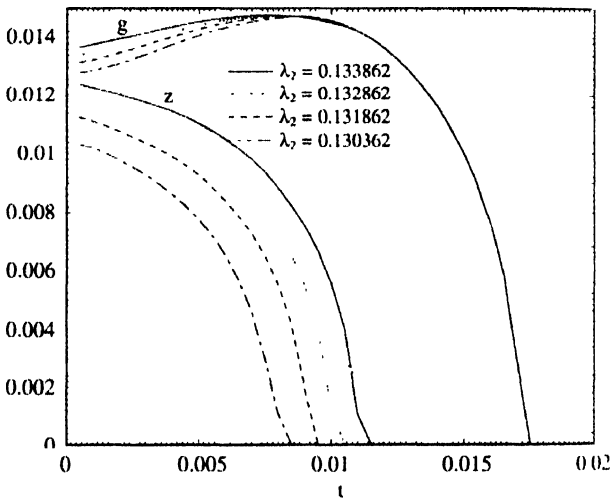

Figure 4. The self-consistent plot of z, g *vs* t for fixed value of $\lambda_1 = 0.238605$ and for different values of $\lambda_2 = 0.133862$, 0.132862, 0.131862, 0.130362

The SDW coupling λ_2 enhances the SC gap parameter through out the temperature range. In the process, SC transition temperature t_c is enhanced. It shows as if the SDW coupling acts as the SC coupling. On the other hand, the SDW coupling constant enhances the SDW gap parameter $g(t)$ in the temperature range where the co-existent phase exists. However, the SDW gap remains unaltered for the temperature $t > t_c$, keeping t_N constant.

(B) Case $T_N > T_c$:

Another set of coupling constants $\lambda_1 = 0.188605$ and $\lambda_2 = 0.130362$ are selected to give the transition temperatures $T_N > T_c$ in their individual phases [see Figure 5].

When the two phases co-exist and interplay each other, the self-consistent solutions of the eqs. (9) and (10) for the above set of parameters give temperature dependences of the SC gap $z(t)$ and SDW gap $g(t)$ as shown in Figure 6.

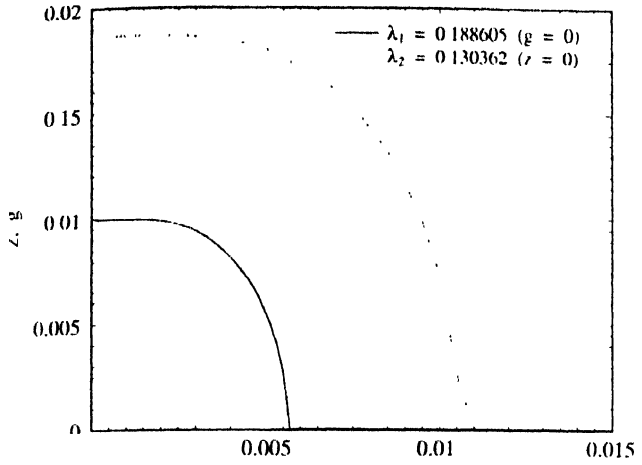

Figure 5. The plot of g *vs* t for fixed values of $z = 0$, $\lambda_1 = 0$, $\lambda_2 = 0.130362$ and the plot of z *vs* t for fixed values of $g = 0$, $\lambda_1 = 0.188605$, $\lambda_2 = 0$.

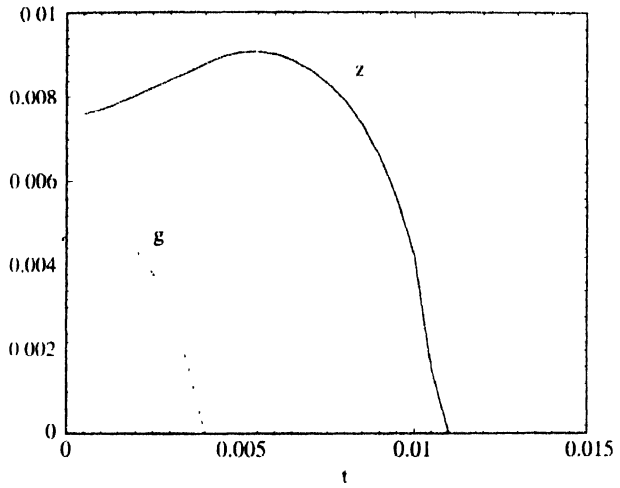

Figure 6. The self-consistent plot of g, z *vs* t for fixed values of $\lambda_1 = 0.188605$ and $\lambda_2 = 0.130362$.

This corresponds to a system with $t_c > t_N$. This situation is realized in the $TmNi_2B_2C$ system with T_c/T_N ~7.33 which is observed experimentally. Both the gap parameters exhibit mean-field temparature dependence. The SC order parameter at the outset increases as the temperature is lowered below t_c, attains a maximum at around $t_c/2$ and there after starts decreasing towords the low temperatures.

The effect of SC coupling constant λ_1 on the temperature dependence of both the gap parameters is shown in Figure 7.

An increase in the SC coupling constant λ_1 enhances both the SDW gap and Néel temperature where as it enhances the SC gap parameter $z(t)$ in the temperature range $t < t_N$ in the co-existent phase. However the gap remains unaltered for the temperature $t > t_N$ keeping t_c constant.

The effect of SDW coupling λ_1 on the SC gap $z(t)$ and SDW gap $g(t)$ is depicted in Figure 8.

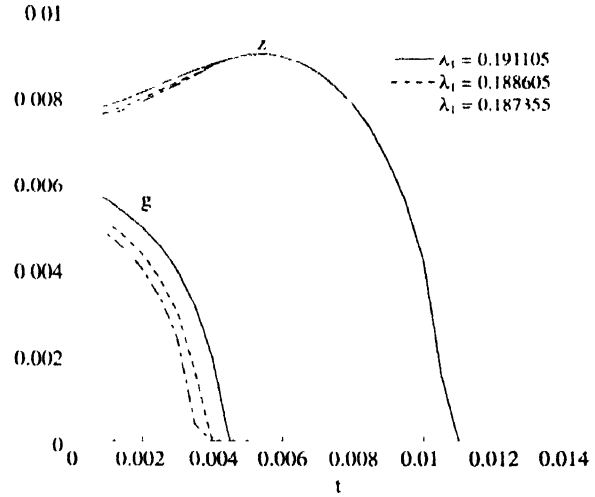

Figure 7. The self-consistent plot of g, z *vs* t for fixed values of $\lambda_2 = 0.130362$ and for different values of $\lambda_1 = 0.191105$, 0.188605, 0.187355.

The SDW coupling λ_2 suppresses the SDW gap through out the temperature range and also suppresses the Néel temperature. The increase of SDW coupling λ_2 enhances the SC gap $z(t)$ through out the temperature range and pushes the SC transition temperature to higher temperatures. It is clear from the Figures 7 and 8 that

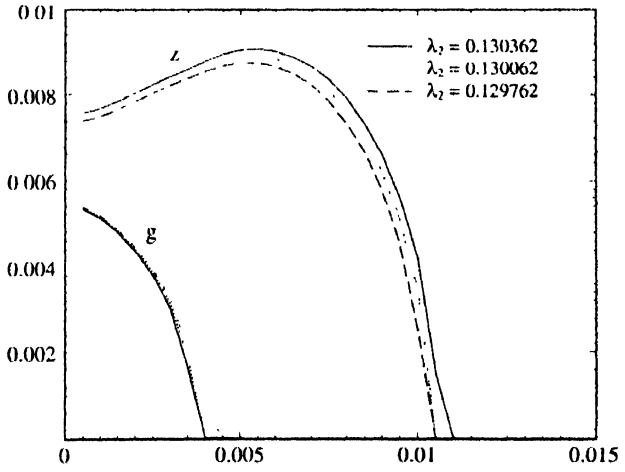

Figure 8. The self-consistent plot of g, z *vs* t for fixed values of $\lambda_1 = 0.188605$ and for different values of $\lambda_2 = 0.130362$, 0.130062, 0.129762.

the roles of the SC coupling λ_1 and SDW coupling λ_2 are reversed. In other words, the SC coupling λ_1 acts as the SDW coupling while the SDW coupling λ_2 acts as the SC coupling.

5. Conclusion

We have considered a model Hamiltonian consisting of BCS type mean field term for superconductivity and the

mean field spin density wave term for the conduction electrons of the borocarbide system. The Hamiltonian is solved for the SC gap parameter and the SDW gap parameter by using Zubarev type Green's function technique. These two gap parameters are solved self-consistently by adjusting the two coupling constants *i.e.* SC coupling λ_1 and SDW coupling λ_2 for the situation $T_c > T_N$ and $T_c < T_N$, appropriate for the general borocarbide systems RNi_2B_2C (R= Lu, Ho, Tm, Dy.....). The numerical solutions show that both the SC and SDW gap parameters exhibit mean field temperature dependence. However one gap parameter shows suppression at low temperatures where the other phase co-exists with it and the *vice-versa*. Moreover, the SC coupling constant acts as the SDW coupling constant and the *vice-versa*. Similar observations are indicated in the communication [23] consisting of a model Hamiltonian containing superconductivity and anti-ferromagnetism arising due to the same conduction electrons and a weak hybridization between the conduction electrons of the nickel atom and the *f*-electrons of the rare-earth atom.

Acknowledgments

One of the authors (GCR) would like to acknowledge the University Grants Commission for the financial assistance. The authors (KCB and GCR) gratefully acknowledge the research facilities offered by the Institute of Physics, Bhubaneswar, Orissa, India during their short stay.

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